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Modeling of Laser Damage Initiated by Surface Contamination

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Abstract

We are engaged in a comprehensive effort to understand and model the initiation and growth of laser damage initiated by surface contaminants. This includes, for example, the initial absorption by the contaminant, heating and plasma generation, pressure and thermal loading of the transparent substrate, and subsequent shockwave propagation, "splashing" of molten material and possible spallation, optical propagation and scattering, and treatment of material fracture. The integration use of large radiation hydrodynamics codes, optical propagation codes and material strength codes enables a comprehensive view of the damage process

The following picture of surface contaminant initiated laser damage is emerging from our simulations.

On the entrance optical surface, small particles can ablate nearly completely. In this case, only relatively weak shockwaves are launched into the substrate, but some particulate material may be left on the surface to act as a diffraction mask and cause further absorption. Diffraction by wavelength scale scattering centers can lead to significant intensity modulation. Larger particles will not be completely vaporized. The shockwave generated in this case is larger and can lead to spallation of contaminant material which then may be deposited in the substrate. A gaseous atmosphere can lead to radiation trapping with concomitant increases in temperature and pressure near the surface. In addition, supersonic ionization waves in air may be generated which greatly extend the plasma plume spatially and temporally.

Contaminants on the exit optical surface behave differently. They tend to heat and pop off completely in which case significant damage may not occur. Since plasma formed at the interface of the optic and absorbing particle is confined, much stronger pressures are generated in this case.

Imaging of contaminants resulting in "writing" a diffraction pattern on the exit surface due to contamination on the entrance surface has been observed experimentally and predicted theoretically. Such imprinted damage regions can seed damage from subsequent pulses.

Introduction

Large high power laser systems under development, such as the National Ignition Facility and the Laser Megajoule, contain many types of optical elements. These elements, lenses, mirrors, debris shields, etc. are made of various substrates with or without various types of coatings. They are designed to work in vacuum or gaseous environments, often vacuum on one side and gas on the other. To contain cost, such systems must operate close to optical damage thresholds. On the other hand, because of the very large number of components, it is necessary to establish safe operational limits and tolerable contamination levels. It would be difficult to establish such limits completely empirically owing to the large number of materials, coatings, environment and the need to scale from small experiments to full sized optical elements. For this reason, it is useful to establish theoretical models of laser induced damage to aid understanding and interpretation of empirical knowledge. A review of theoretical models of laser damage in transparent materials is given by ref. [1].

Our initial effort to understand quantitatively the interaction of high power lasers with surface contaminants is the subject of the present paper. The theoretical description must include optical propagation, absorption and ionization of material, hydrodynamics and shock wave propagation, thermal and radiation transport, elastic-plastic material response and material failure. No computational model at present contains all of the necessary physics. However, we have coordinated several powerful computer codes to extend our understanding of the laser damage regime. In combination with carefully designed experiments, modeling can identify significant physical effects and scaling behavior.

Below we discuss several important physical effects accompanying laser interaction with metallic surface contaminants. Comparing the results of experiment and modeling, we address the following questions. First, what difference does it make if the contaminant is on the entrance or exit surface?. What is the connection between plasma generation and damage? What is the effect of the surrounding environment? Finally, a summary of our results and a list of outstanding questions is given.

Physical Effects

Optical surfaces can be contaminated by small particles, say tens to hundreds of micrometers in size. These arise, for example, from dust, condensation, debris from light interaction with chamber walls and targets. Various types, sizes and shapes of contaminant should be studied. For definiteness and reproducibility, experiments and modeling in the present work refer to artificial "particles" deposited on a silica substrate. These 1 μm thick particles of C, Al or Ti are sputter deposited through a mask and can be either round or square in shape.

For metallic particles, laser light is absorbed in a thin skin depth leading to strong heating and plasma formation. The temperature of the resulting plasma can be as high as 20eV resulting in multiple ionization of the material. Such a hot plasma is a strong radiator of UV and soft x-rays. In this case, radiation transport dominates thermal conduction as a means of transporting energy. This radiation is strongly absorbed in any surrounding air causing heating and further ionization. In this case, the ionization front in the air can expand supersonically as we will see below. UV emission from the plasma can also be absorbed in the substrate, creating color centers which increase absorption seen by subsequent pulses.[2] The strongly localized energy deposited in the substrate produces strong shock waves which can cause mechanical damage. Finally, the plasma radiation can induce electronic defects in the glass which permanently change its absorption and decrease the damage threshold for subsequent pulses.

It has long been noted that laser damage usually is easier to induce on the exit surface. Conventional wisdom [3 points to Fresnel reflection as the source of this asymmetry. However, the predicted ratio of thresholds does not always hold. Further, this effect should vanish for AR coated optics. We wish to point out another difference between contaminated entrance and exit surfaces. On the entrance surface, the plasma formed expands and shields the particle from the incoming laser light. That is, further laser energy is absorbed in the plasma itself. Consequently, the pressure pulse launched into the substrate is on the order of 10 kbar. On the exit surface, the plasma is formed at the interface of two solid materials and confined. The high density of the plasma means higher heat capacity, lower temperature and much higher pressures (say 60 kbar).

Numerical Models

The interaction of laser light with matter on a nanosecond time scale is described by the radiation-hydrodynamics codes HYADES(1D) [4] and LASNEX(1D or 2D) [5], respectively. These codes regard materials as fluids described by empirically based equations of state and opacities. The codes account for material ionization, radiation emission and absorption, nonlinear hydrodynamics including shock waves, and radiation and electron transport. The codes have no description of shear stresses or final strength of materials. They cannot describe mechanical deformation and failure.

However, such deformation and failure occur on a time scale very long compared to the laser pulse durations of 20 ns considered here. The deformation therefore also takes place in a volume large compared to the laser material interaction volume. Thus, the laser-matter interaction nearly decouples from the subsequent thermo-mechanical material response. We can use the pressure pulse from the radiation-hydrodynamics modeling as a boundary condition for materials codes.

This is the approach we have taken using the DYNA[6] and CALE[7] codes which describe elastic-plastic response and material failure, but do not include a description of the laser matter interaction. Thermal transport in complex situations is treated by the TOPAZ[8] code.

Results

In one set of experiments, the artificial particle was irradiated by a single 5 ns damaging pulse together with a 20 ns weak probe pulse. The particle was imaged in the probe light onto the entrance slit of a streak camera to obtain a time history. A more complete description of the experimental setup will be given elsewhere. A typical experimental streak for a 150 μm Al "dot" on the exit surface in air is shown in Fig.[1]. Here time advances down the vertical axis. The bright background is the light of the probe pulse and the initial dark region is the obscuration due to the dot. The damaging pulse is turned on approximately from 20-25 ns during which time the obscured region begins to grow. It continues to grow at a supersonic rate of more than 10 $\mu m/ns$ after the damaging pulse is over. Very different behavior was noted for surfaces in vacuum. In this case, the obscuration stops growing after the end of the damaging pulse.

In a second series of experiments, the particle was subjected to multiple pulses with wavelength of either 1064 or 355 nm. Particles on the entrance surface were tended to melt/vaporize and redeposit. The redeposited material served as absorbing centers for later pulses and substantial damage. Particles on the exit surface were more likely to pop off without causing serious damage. This may be due to the extreme thinness of our pancake like particles. The effect of aspect ratio will be investigated in future work. One of the most interesting results was the observation that a contaminant particle on the entrance surface can "write" its diffraction pattern on the exit surface (see below).

The presence of a gaseous atmosphere tends to retard the plasma expansion. More significantly, UV emission from the plasma is absorbed in surrounding air as shown in Fig. 2. This calculation refers to an Al particle on the front surface in air. Initial absorption in the Al leads to a hot (10eV) localized plasma. By the peak of the pulse (t=5 ns) a layer of hot air has formed in front of the Al plasma due to plasma emission. At later times (t=13 ns) the layer of heated and ionized air continues to grow at an expansion rate on the order of 20 $\mu m/ns$. Such trapping is expected for photons with energy above about 5 eV since their mean free path is less than 100 μm[9]. The radiation trapping leads to higher temperature and slightly higher pressure than would occur in vacuum.

Much stronger confinement occurs when the particle is on the exit surface since the plasma now forms between the particle and the substrate. In this case, as shown in Fig.(3) for time t=5 ns, peak pressures on the order of 50-60 kbar occur in contrast to the typical value of 10 kbar for front surface particles. This strong pressure tends to pop particles off the exit surface as shown by the density plot in Fig. 4. Here the laser beam comes from below (positive z values), the 4 μm thick Al particle flies off the surface and densification occurs behind the shock wave launched into the substrate. We find, as expected, that higher pressures build up with thicker particles.

We have used the pressure and temperature loadings calculated above as input to the material response codes to model elastic-plastic and thermal response of the substrate materials. For example, Fig. 5 illustrates the damage pattern in a glass substrate (simple yield stress) resulting from laser absorption in a spherical Al particle on the front surface. Our calculations of surface particle spallation, shock hardening, crack growth and thermal expansion induced stresses show sensitivity to material properties such as the thermodynamic equation of state, temperature dependence of light absorption and material strength models. We are presently improving the physical models and material values used in these codes. In addition, the initial laser-matter calculations are being extended to two spatial dimensions for assessment of edge effects.

In our experiments, we observed damage patterns on the exit surface attributable to contamination of the front surface. In the clearest cases, occurring at wavelength 355 nm in a range of fluences below the nominal damage threshold, an image of the front surface particle is written on the exit surface. A typical example is shown in Fig 6 where a rear surface pattern (Nomarski microscope) is shown corresponding to a round 150 μm particle on the front surface. The thickness of the substrate is 11 mm. The experimental pattern, reminiscent of the "spot of Arago" of optics texts, is completely explainable as the material response to simple diffraction around the original obstacle(Fig. 7. At the thicknesses of substrate (1 cm) used here, self-focusing should not play a role so the "writing" of this image once again points out the special vulnerability of the exit surface to laser damage.

Conclusions

We have combined numerical models of laser absorption, plasma generation, radiation-hydrodynamics and thermal-mechanical material response to obtain a unified treatment of surface initiated laser induced damage. In conjunction with experiments, modeling indicates the importance of radiation confinement by either air (front surface) or contaminant (rear surface). Higher pressures are obtained with rear surface contaminants which are also more likely to "pop off". Front surface contaminants can result in rear surface damage through simple diffraction around opaque particles. This work was performed under the auspices of the U.S. DOE by LLNL under contract number W-7405-Eng-48.

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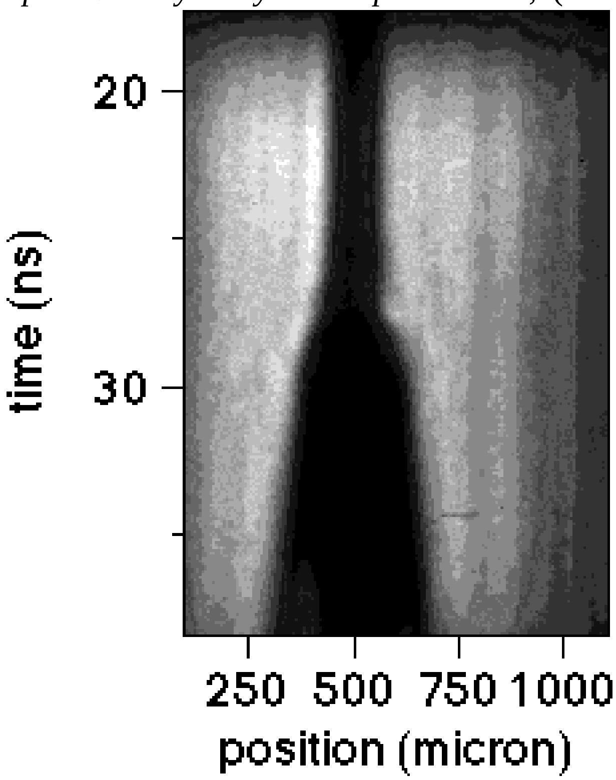


fig 1

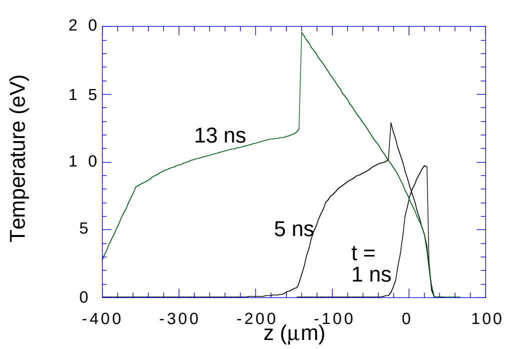


Fig. 2

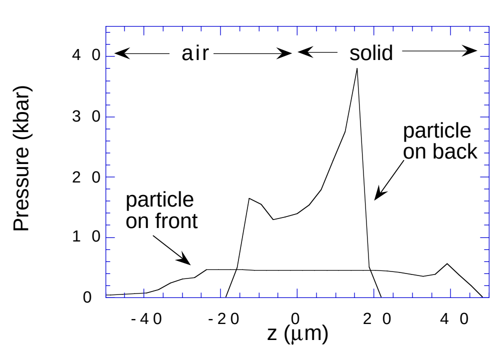
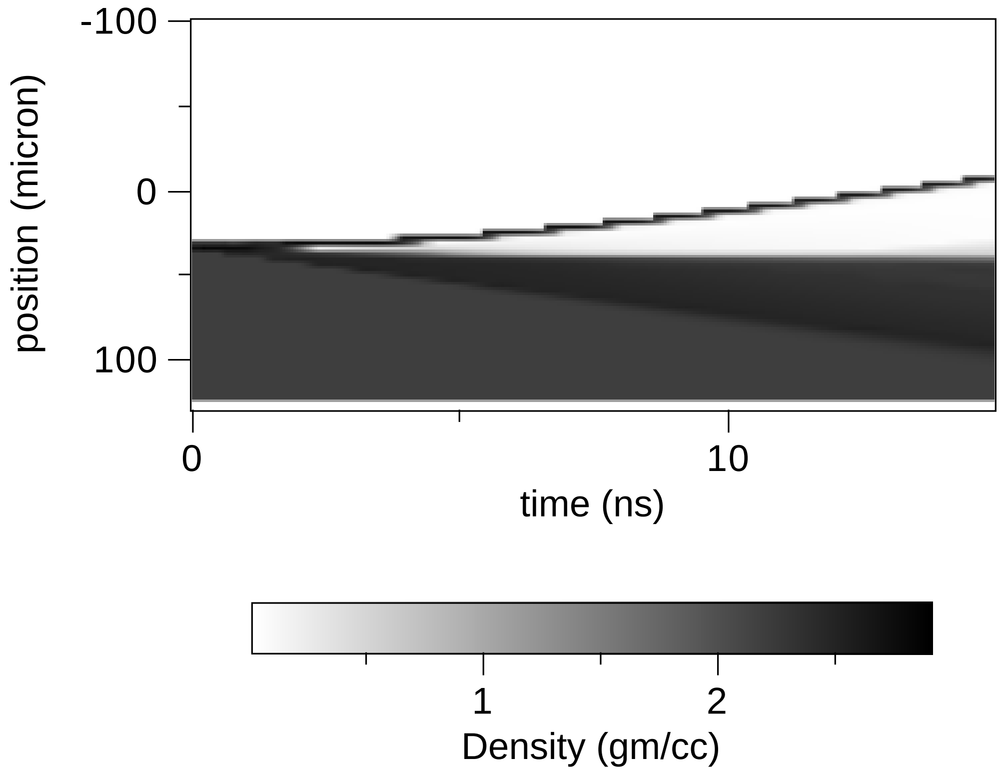


Fig. 3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0
100
position (micron)
0
10
time (ns)
1
2
Density (gm/cc)

Fig. 4

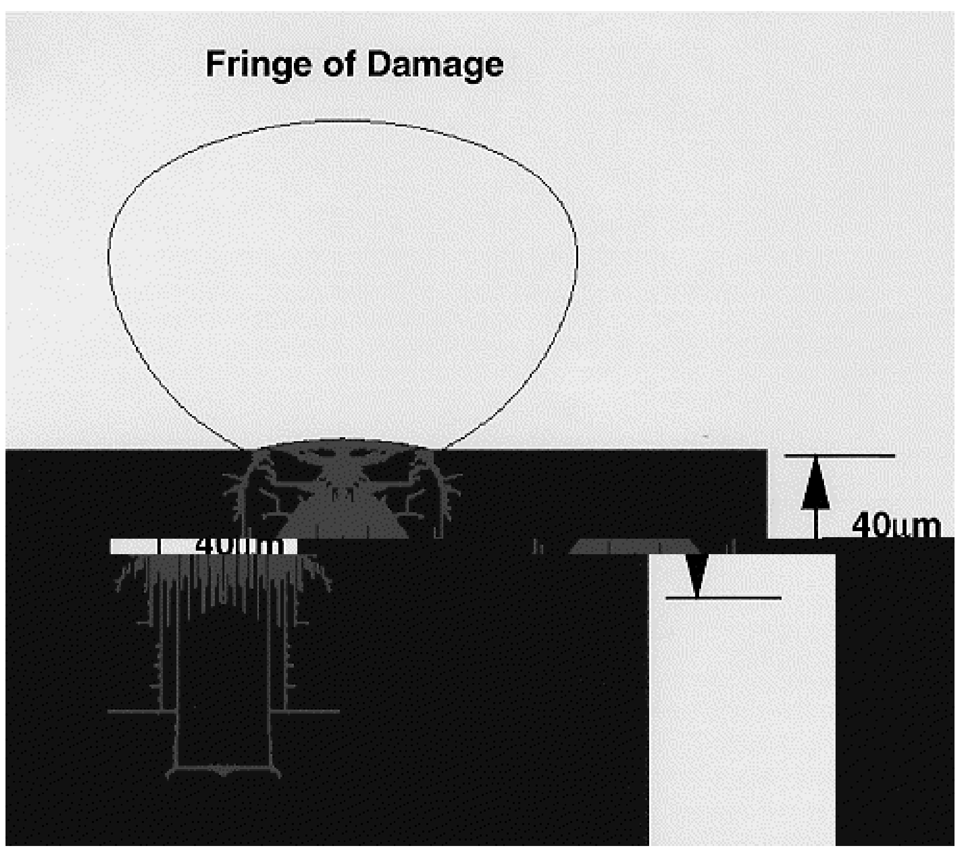
Fringe of Damage
40μm

Fig. 5

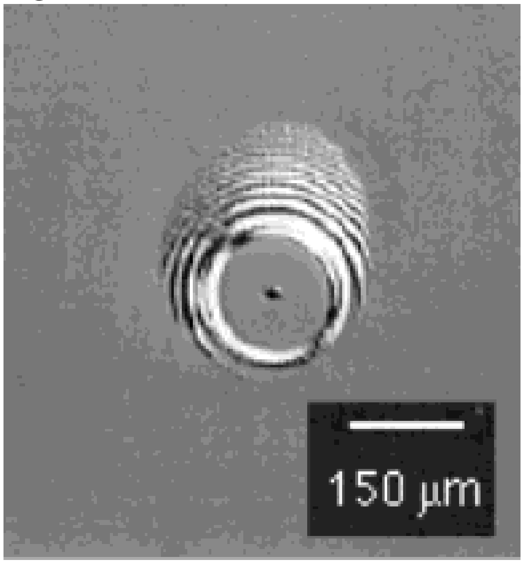

Fig. 6

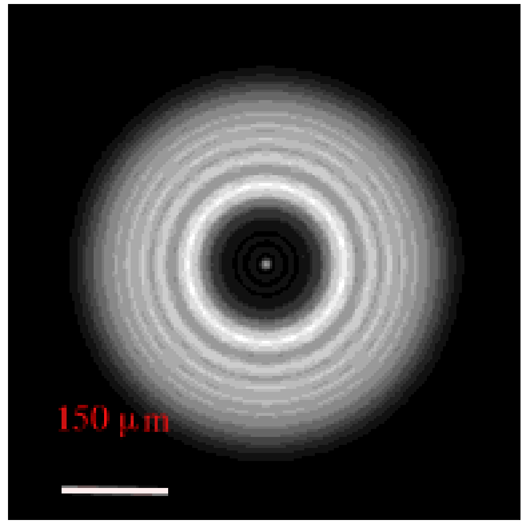

Fig. 7